Spectral Flow and the Dynamics of Dislocations in Charge Density Waves

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The spectral flow in the cores of moving dislocations is found to play an important role in the dynamics and transport of charge density wave (CDW) by significantly modifying the hydrodynamic effective action of the condensate. The analogy of spectral flow in CDW with the baryogenesis in the early universe is pointed out.

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The dynamics of the dislocation lines in charge density waves (CDW's) [1] is one of the key processes which govern the sliding (nonlinear) conductance of the incommensurate CDW with three dimensional (3D) order. When current contacts are attached to the side of the chains, a sliding CDW implies that wave fronts are added or removed at the contacts by the nucleation or annihilation of dislocation loops as shown in Fig. 1. The narrow band noise [2,3] and the nonlinear current-voltage characteristics [4–8] have been attributed to this phenomena. Although this idea explains most qualitative features of CDW very well, the dynamics of the dislocations is not yet well understood. Especially, the gauge invariance or charge conservation condition of CDW has not been investigated seriously.

In this Letter, we first show that the gauge invariance of the conventional hydrodynamic effective action of the condensate is violated in the presence of moving dislocations. The origin of this is shown to be the neglect of the "spectral flow" in the cores of the moving dislocations. By explicitly taking the effects of the spectral flow into account, we derive a gauge invariant action which correctly describes the dislocation dynamics. We find two correction terms arising from the spectral flow, namely, the correction to the interaction of the condensate with the electromagnetic field and to the condensation energy. The nucleation process of the dislocation loop is analyzed based on the obtained action and the nonlinear conduction of the CDW is discussed in the light of our findings. Finally we discuss a remarkable similarity of the dislocations in CDW with the so-called cosmic strings in the early universe, suggesting the intriguing possibility of the CDW system as a theoretical and experimental model for cosmological field theories.

First we discuss the gauge invariance of the effective action in the presence of moving dislocations. It has been widely accepted that the condensate can be described by a hydrodynamic action, which is valid on a length scale larger than ξ_α's [9], with ξ_α being the amplitude coherence length ($\alpha = x, y, z$ depending on the direction). The action consists of the elastic part $S_{\rm el}$ and the interaction part with the electromagnetic field $S_{\rm int}$,

$$S = S_{\rm el} + S_{\rm int} \tag{1}$$

$$S_{\rm el} = \int d\tau d\mathbf{r} \frac{K}{2} \Big\{ c_0^{-2} \left(\partial_\tau \theta\right)^2 + \left(\partial_x \theta\right)^2 + \gamma_y^2 \left(\partial_y \theta\right)^2 + \gamma_z^2 \left(\partial_z \theta\right)^2 \Big\} \tag{2}$$

$$S_{\rm int} = \int d\tau d\mathbf{r}\; iL \left(\varphi \partial_x \theta + A_x \partial_\tau \theta\right) \tag{3}$$

where $\theta(\tau, \mathbf{r})$, $\varphi(\tau, \mathbf{r})$ and $A_x(\tau, \mathbf{r})$ are the phase of the order parameter, the scalar potential and the x-component of the vector potential, respectively. $\mathbf{r} = (x, y, z)$ and τ is the imaginary time. The conducting chains are parallel to the x-axis. $K = N_\perp f_{\rm c} \hbar v_{\rm F}/2\pi$ and $L = eN_\perp f_{\rm c}/\pi$, where $f_{\rm c}$, $v_{\rm F}$, $N_\perp$ are the condensate fraction, the Fermi velocity parallel to the chains and the areal density of the chains, respectively. $c_0 = v_{\rm F}\sqrt{m/m^*}$ is the phason velocity with m^*/m being the effective mass ratio of the condensate to the normal electrons. $\gamma_y (= \xi_y/\xi_x)$ and $\gamma_z (= \xi_z/\xi_x)$ are the anisotropy parameters.

According to the action, Eq. (3), the charge density $\rho_{\rm c}(\tau, \mathbf{r})$ and current density $\mathbf{j}_{\rm c}(\tau, \mathbf{r})$ of the condensate are expressed by,

$$\rho_{\rm c} = L\partial_x \theta, \quad \mathbf{j}_{\rm c} = -L\; \hat{\mathbf{e}}_x\; \partial_\tau \theta, \tag{4}$$

where $\hat{\mathbf{e}}_x$ is the unit vector parallel to x-axis. The charge conservation law then reads,

$$L \left(\partial_\tau \partial_x \theta - \partial_x \partial_\tau \theta\right) = \Gamma_{\rm qp}. \tag{5}$$

Although $\Gamma_{\rm qp}(\tau, \mathbf{r})$ vanishes when $\theta(\tau, \mathbf{r})$ is a single valued smooth function of τ and $\mathbf{r}$, it does not vanish in the presence of moving dislocations [10] and gives [11]

$$\Gamma_{\rm qp} = -2\pi L \sum_\nu \int dl \left(\partial_l \mathbf{R}_\nu \times \partial_\tau \mathbf{R}_\nu\right)_x \delta^{(3)}(\mathbf{r} - \mathbf{R}_\nu), \tag{6}$$

where $\delta^{(d)}(\mathbf{r})$ and $\mathbf{R}_\nu(\tau, l)$ are the d-dimensional δ-function and the positions of the ν-th dislocation line at imaginary time τ, respectively. l is a parameter along the

line. In this Letter we consider only the dislocations with 2π phase singularity and those with higher (4π, $6\pi\cdots$) singularities are disregarded because of the higher excitation energies. The Eq. (6) clearly shows that charge conservation is violated in the cores of the dislocations, and implies the conversion of the quasiparticles into condensate electrons. Although this phenomenon has been discussed earlier by several authors [3,12], its effects on the effective action of the dislocations have not been considered.

The origin of $\Gamma_{\rm qp}$ becomes clearer by examining the energy spectrum of the quasiparticles in the core region. We consider chains of a finite length l_x ($0 < x \le l_x \equiv 1$) and assume that a straight dislocation line parallel to the z-axis is moving from $y = 0$ to $y = l_y$ along the plane $x = l_x/2$. (See Fig. 2 (a).) We calculate the energy spectrum of the chain located at $y = l_y/2$. The complex order parameter, $\Delta(\tau, \mathbf{r})$, on the chain is parameterized as $\Delta(x, Y_v)$, where Y_v is the y-coordinate of the dislocation line. The anisotropy of the system and the interchain electron hopping is neglected for simplicity. We take $\Delta(x, Y_v)$ to be constant at $x = 0$, 1, by assuming perfect pinning at the ends of the chains. $\Delta(x, Y_v)$ must be quasiperiodic in Y_v, $\Delta(x, Y_v) \propto \exp(-2\pi i x)\ \Delta(x, Y_v + l_y))$, corresponding to the addition of a wave front of CDW due to the dislocation [13]. By numerically diagonalizing the Hamiltonian,

$$\mathcal{H} = \int dx\ \Psi^\dagger \cdot \begin{pmatrix} -\hbar v_{\rm F} i\partial_x & \Delta(x, Y_v) \\ \Delta^*(x, Y_v) & \hbar v_{\rm F} i\partial_x \end{pmatrix} \cdot \Psi, \qquad (7)$$

where $\Psi = (\mathcal{R}(x), \mathcal{L}(x))$ with $\mathcal{R}(x)$ and $\mathcal{L}(x)$ being the field operators for right and left moving electrons omitting the spin degree of freedom, we obtain the energy spectrum of the quasiparticles shown in Fig. 2 (b). It clearly shows the spectral flow phenomenon; one energy level is transferred from above to below the energy gap through the core of the dislocation. When the energy level is occupied (vacant) at $Y_v = 0$, a quasielectron in the conduction band (quasihole in the valence band) is deleted (created) during this process. Since this process is strongly localized to the cores of the dislocations, the size of which is given by the amplitude coherence length ξ_α's, it cannot be described by the conventional hydrodynamic effective action of the condensate which is valid on a scale larger than ξ_α's.

Our next task is to derive the effective action of the condensate which correctly describe the spectral flow in the cores of dislocations. We found that two correction terms to Eq. (3) are needed. One is the correction term to the electromagnetic interaction, $S_{\rm int}$, and the other is related to the change of the total condensation energy by the spectral flow. The former should be introduced to compensate the violation of the gauge invariance discussed above. We first focus on a single chain to analyze this situation. The motion of a dislocation is then a phase slip process localized at the core [12]. The quasiparticles are created at this position and diffuse over the entire chain. The number of created quasiparticles is two (including the spin degree of freedom) at 0 K, and decreases at higher temperatures in proportion to the equilibrium condensate fraction $f_{\rm c}$. The actual diffusion process of the quasiparticles is governed by the mobility, which depends on the material. In a dirty CDW sample, the motion of the quasiparticles is diffusive, whereas in a clean one it can be ballistic. The situations are classified by the relation between the quasiparticle velocity $v_{\rm qp}$ and the phason velocity c_0. The latter characterizes the velocity of the propagation of deformations in the condensate. The following two limiting cases are useful.

Clean limit ($v_{\rm qp} \gg c_0$) — Since the effective mass of the quasiparticles near the energy gap can be approximated by $m_{\rm eff} \simeq \Delta_0/v_{\rm F}^2$, where Δ_0 is the equilibrium energy gap, an applied field accelerates the quasiparticles to $v_{\rm qp} = \sqrt{e\Delta_0/m_{\rm eff}} = v_{\rm F}$ without impurity scattering. (The particle-hole process limits the speed.) Since $v_{\rm F} \gg c_0$ the quasiparticles move much faster than the condensate in this limit. Then the spatial change in the quasiparticle current density at the dislocation position can compensate $\Gamma_{\rm qp}$ in Eq. (5) and the correction can be implemented by introducing the following term to the effective action,

$$\delta S_{\rm int} = -iL \int d\tau d\mathbf{r}\ A_x(\tau, \mathbf{r}) \int^x dx'\ \Gamma_{\rm qp}(\tau, x', y, z)\,. \qquad (8)$$

Dirty limit ($v_{\rm qp} \ll c_0$) — With impurity scattering, $v_{\rm qp}$ is given by $-\mu_{\rm qp}E_x$, where E_x and $\mu_{\rm qp}$ are the applied field and quasiparticle mobility, respectively. When $v_{\rm qp}$ is much smaller than c_0 it is a good approximation to neglect the motion of the created quasiparticles. Then the correction term becomes,

$$\delta S_{\rm int} = iL \int d\tau d\mathbf{r}\ \varphi(\tau, \mathbf{r}) \int^\tau d\tau'\ \Gamma_{\rm qp}(\tau', \mathbf{r})\,. \qquad (9)$$

For example, if the mobility is of the order of $\sim 1{\rm cm}^2/{\rm V\cdot s}$, which is a typical value for the conventional samples, $v_{\rm qp}$ is smaller than c_0 unless $E_x > 10^6{\rm V/cm}$, which is much larger than the experimental value. The dirty limit therefore applies to most of conventional CDW samples.

The second correction term arises from the condensation energy. The dislocation motion in CDW always produces quasiparticles from the condensate. If some quasiparticles already exist near the dislocation core, the dislocation can convert some to the condensate and gain condensation energy. Employing Eq. (6), the contribution of the condensation energy to the effective action of the dislocation is estimated as $\delta S_{\rm cd} \sim \pm \int d\tau d\mathbf{r} (\Delta_0/e) \int^\tau d\tau' \Gamma_{\rm qp}(\tau', {\rm r})$, where $\pm$ depends on the situations described above. In most CDW materials,

Δ_0/e is of the order of 0.1 V and is important, especially when the x-component of the applied electric field is small (for example, in a transverse field condition [14]).

Next we discuss the effective action of the dislocations taking into account the correction derived above. It is convenient to transform here to an isotropic coordinate system by $x = (x_0, x_1, x_2, x_3)$ with $x_0 = c_0\tau$, $x_1 = x$, $x_2 = y/\gamma_y$, $x_3 = z/\gamma_z$, $\tilde{K} = K\gamma_y\gamma_z/c_0$ and $\tilde{L} = L\gamma_y\gamma_z/c_0$. We express $\partial_\mu\theta$ in terms of the dislocation coordinate since $\partial_\mu\theta$ is well-defined and single valued, although θ itself is not. As in Eq. (6), we parameterize the position of the ν-th dislocation in space and time by l and τ, respectively. The position of the line element in 4D space is expressed by $\eta_\nu(\tau, l) = (c_0\tau, \mathbf{R}_\nu) = (c_0\tau, X_\nu, Y_\nu, Z_\nu)$. Introducing a flux tensor, $\mathcal{F}_{\alpha\beta}(x)$ [15],

$$\mathcal{F}_{\alpha\beta}(x) = 2\pi \sum_\nu \int dl d\tau \; (\dot{\eta}_\nu)_\alpha (\eta'_\nu)_\beta \delta^{(4)}(x - \eta_\nu), \quad (10)$$

where $\dot{\eta}_\nu \equiv \partial_\tau \eta_\nu$ and ${\eta'}_\nu \equiv \partial_l \eta_\nu$, we obtain

$$\partial_\mu\theta(x) = \int d^4x' \epsilon_{\mu\alpha\beta\gamma}\partial_\alpha G^{(4)}(x - x')\mathcal{F}_{\beta\gamma}(x'), \quad (11)$$

where $G^{(4)}(x) = -(4\pi^2)^{-1}|x|^{-2}$ is the Green's function of $-\partial_\mu\partial_\mu$ and $\epsilon_{\mu\alpha\beta\gamma}$ is the fully antisymmetric tensor. Here the single valued part of θ is omitted. Employing Eq. (11) we can express all the terms in terms of $\mathbf{R}_\nu(\tau, l)$. For example, $S_{\rm el}$ of Eq. (3) is rewritten as,

$$S_{\rm el} = \int d^4x d^4x' \; \frac{\tilde{K}}{2} \; G^{(4)}(x - x')\mathcal{F}_{\alpha\beta}(x)\mathcal{F}_{\alpha\beta}(x'), \quad (12)$$

where the conservation law of the topological charge of the dislocations, $\partial_\alpha \mathcal{F}_{\alpha\beta} = 0$ [15], has been used.

Now we consider the sliding of CDW by the nucleation of dislocations near the contacts [4,6,7]. The effective action discussed above depends on the electric field in the sample, which is conventionally assumed stationary and parallel to the chains. The "two fluid approximation" yields

$$(-\partial_x^2 + \lambda_0^{-2})E_x = 4\pi D^{-1} \left\{\mathbf{j}_{\rm qp}\right\}_x, \quad (13)$$

where $\lambda_0^{-2} = 8e^2 f_{\rm c}/(\hbar v_{\rm F})$, D and $\{\mathbf{j}_{\rm qp}\}_x$, are the Thomas-Fermi screening length of the normal state, the diffusion constant and the x-component of the quasiparticle current, respectively. From this equation we can see that the electric field distribution depends on $\mathbf{j}_{\rm qp}$ and D, in other words, on the density and mobility of the quasiparticles.

The thermal and quantum nucleation rate of a dislocation loop in the presence of an applied electric field can now be estimated based on the effective action derived above. We employ the method by Langer and Fisher [16,4,7] and by Duan [6], to estimate the thermal and quantum nucleation rate, respectively. In the latter case we take the bounce solution of a dislocation loop as $\eta(\tau, \vartheta) = (c_0\tau, X, \sqrt{R^2 - (c_0\tau)^2}\cos\vartheta, \sqrt{R^2 - (c_0\tau)^2}\sin\vartheta)$, $(0 \leq \vartheta < 2\pi)$, and use the instanton method.

According to the above arguments we can distinguish between the clean and dirty samples and between the metallic and semiconducting materials, which leads to the following picture.

(1) In *clean systems*, in which the quasiparticle motion is ballistic, $\delta S_{\rm int}$ of Eq. (8) must be employed. In this case the dislocations behave like an array of electric dipoles with moments aligned perpendicular to the chains [14] which do not couple with E_x. Therefore the nucleation of the dislocation loop does not lead to a gain of electrostatic energy. In addition, since the deviation of the quasiparticle density from the equilibrium is small, the gain of condensation energy is also negligible. The nucleation of the dislocation loops is then unlikely in these systems and sliding CDW transport is suppressed.

(2) In *dirty metallic systems*, $S_{\rm int}$ in Eq. (3) is modified by Eq. (9) to

$$\begin{aligned} S'_{\rm int} &= S_{\rm int} + \delta S_{\rm int} \\ &= i\tilde{L}\int d^4x \; \Big\{\varphi(x)\int^{x_0} dx'_0 \; \partial_1\partial'_0\theta(x'_0, \mathbf{x}) \\ &\qquad + c_0 A_x(x)\partial_0\theta(x)\Big\} \quad (14) \\ &\approx \frac{i\pi\tilde{L}}{2}\Sigma_\nu \int dx_0 \int dl \, (\mathbf{R}_\nu \times \partial_l \mathbf{R}_\nu)_x \, V(X_\nu), \quad (15) \end{aligned}$$

where $\partial_1 \equiv \partial/\partial x_1$, $\partial'_0 \equiv \partial/\partial x'_0$ and $\mathbf{x} = (x_1, x_2, x_3)$. In the last equation an approximation $c_0 \to \infty$ is applied, which yields $G^{(4)}(x) \to -(4\pi)^{-1}\delta(x_0)|\mathbf{x}|^{-1}$ and the gauge is fixed as $A_x = 0$. $V(X_\nu)$ is given by $\int_0^{l_x} dx_1 \; {\rm sgn}(x_1 - X_\nu)E_x(x_1)$. Note from Eq. (15) that $S'_{\rm int}$ is proportional to the area surrounded by the loop. In this case E_x is approximately constant ($\sim V/l_x$) in the entire sample, where V is the applied voltage.

Since the driving force of the dislocation is strongest near $x_1 = 0$ and $x_1 = l_x$, the nucleation of dislocation loop is most likely to occur at the edges. The effect of the boundary at $x_1 = 0$ (or l_x) can be taken into account by considering mirror dislocations with respect to the boundaries, which replaces $V(X_\nu)$ with $V^b(X_\nu) = 2\int_{X_\nu}^{l_x} dx_1 \;\; E_x(x_1)$ $(= 2\int_0^{X_\nu} \cdots)$ in case of $X_\nu \sim 0$ $(\sim l_x)$. The nucleation rate is then found to be proportional to $\exp\{-(V_{\rm Q}/V)^2\}$ for quantum nucleation, where $V_{\rm Q}^2 = (\pi^2/12)\sqrt{m^*/m}\hbar^3\gamma_y\gamma_z v_{\rm F}^2 f_{\rm c} N_\perp e^{-2}$, and $\exp(-V_{\rm T}/V)$, for thermal nucleation, where $V_{\rm T} = \pi\gamma_y\gamma_z f_{\rm c} N_\perp(\hbar v_{\rm F})^2/(ek_{\rm B}T)$. $V \approx |V^b(X_\nu)|$ is the applied voltage.

(3) In *dirty semiconducting systems*, the same action as Eq. (15) applies. However, since $\mathbf{j}_{\rm qp} \sim 0$ in Eq. (13), E_x in the bulk can be much smaller than V/l_x due to

the screening by the condensate, which reduces the nucleation rate. This qualitatively agrees with experiments [8,17]. Since the quasiparticle density is also strongly modulated, $\delta S_{\rm cd}$ becomes important, which causes a deviation of the nonlinear I-V characteristics from the metallic cases when $V < \Delta/e \simeq 0.1$ V.

The result obtained in (2) coincides with those obtained earlier [4,7] in a different framework, which appears to be accidental however. These theories attribute the driving force of the dislocations to the elastic stress induced in the condensate by the applied electric field, which would imply the unlikely scenario that dislocations nucleate when an electric field is applied without contacts. From our theory it is clear that by nucleation of dislocations no energy is gained in the above situation, since it just results in an over-screening by the condensate. This demonstrates that our theory describes the screening and transport properties correctly.

Before concluding this Letter, we comment on the similarity of the CDW system with field theories for the early universe. A dislocation in CDW is a counterpart of a cosmic string, *i.e.* a topological defect in electroweak field; The former creates quasiparticles from the condensate (Fermi sea) without creating anti-quasiparticles as is clear from Fig. 2, whereas the latter produces matter without producing antimatter, which is called baryogenesis [18,19]. Although the similarity of baryogenesis with the momentum creation in the vortices in superfluid He3 has already been discussed [20], the CDW system is more similar to the electroweak theory in the sense that it has an identical chiral symmetry and chiral anomaly [21]. We therefore expect that further theoretical and experimental studies of CDW may shed new light on its field theoretical counterpart in particle physics and cosmology.

In conclusion, we studied the dynamics of the dislocations in CDW's taking into account the contribution of the spectral flow in the cores. Our theory not only provides a natural basis to understand the dynamics of the dislocations in CDW's but also indicates new aspects of CDW.

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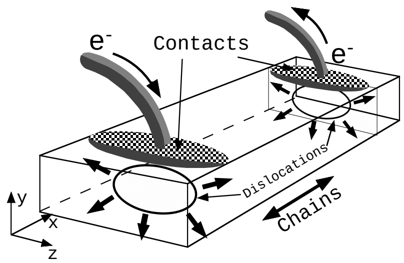

FIG. 1. A schematic view of the nonlinear conductivity measurement. Wave fronts are indicated by shades. Dislocation loops and their motions are shown.

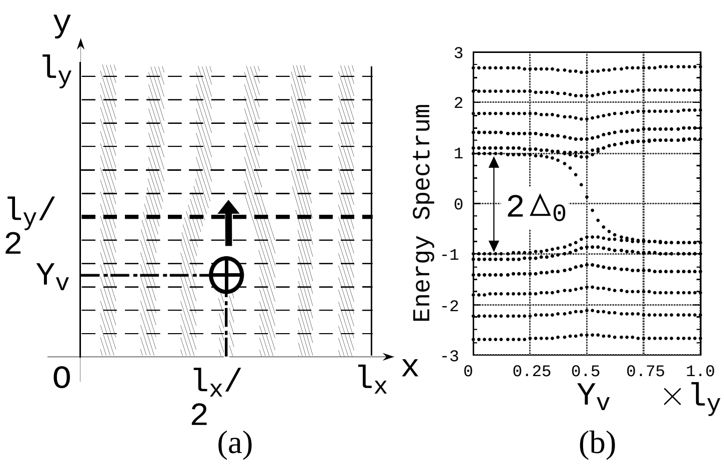

FIG. 2. (a) The configuration of the dislocation ($\oplus$), the chains (dotted lines) and wave fronts (shades). (b) The energy spectrum of a chain (bold line of (a)) as a function of the position of the dislocation, Y_v, is shown. All the energy levels are doubly degenerated at $Y_v = 0, l_y$ except for the innermost two with respect to the energy gap at $Y_v = 0$. In this calculation $\xi = 0.1$ is taken.